

Tris(2-chloroisopropyl)phosphate
13674-84-5 | DTXSID5026259

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 8.84

Global applicability domain: Inside

Local applicability domain index: 9.56e-01

Confidence level: 8.42e-01

Nearest Neighbors from the Training Set

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1,2,4-Trichlorodibenzo-1,4-dioxin

Measured: 8.97

Predicted: 8.77

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4,4'-Dibromodiphenyl ether

Measured: 8.64

Predicted: 8.53

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2,3,7-Trichlorodibenzo-p-dioxin

Measured: 9.14

Predicted: 8.95

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1,2,3,5,7-Pentachloronaphthalene

Measured: 8.82

Predicted: 8.95